# A NEW CHIRAL ALLOTROPE $C_{80}$

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## ABSTRACT

The theoretical prophecy is given on a new chiral allotrope of Fullerene–$C_{80}$. $C_{80}$ molecuule should have 3 $C_2$ symmetric axes, which should be vertical each other. $C_{80}$ should have two chiral allotropes. $^{13}$C-NMR spectra of $C_{80}$ should consist of 20 lines of equal intensity.

**Keywords** $C_{80}$, Fullerene, Chiral allotrope

The double-helical construction of $C_{76}$ chiral allotrope[1] was reported. For researching the chiral origin of the Fullerene molecules, it is tried to make a $C_{76}$ model according to the drawing of the structure II illustrated in Fig.3b of Ref.[1]. A $C_{76}$ model could not be gotten, but only an incomplete polyhedron. For closing it, two six-membered rings (6MR) must be filled on the two opposite symmetric places of the molecule model. On the basis of the definition of Fullerene: a closed, hollow network of 12 pentagonal and m hexagonal rings for a $C_{20+2m}$ molecule,[1] here $m$ is 30, so the new Fullerene molecule should be $C_{80}$ .

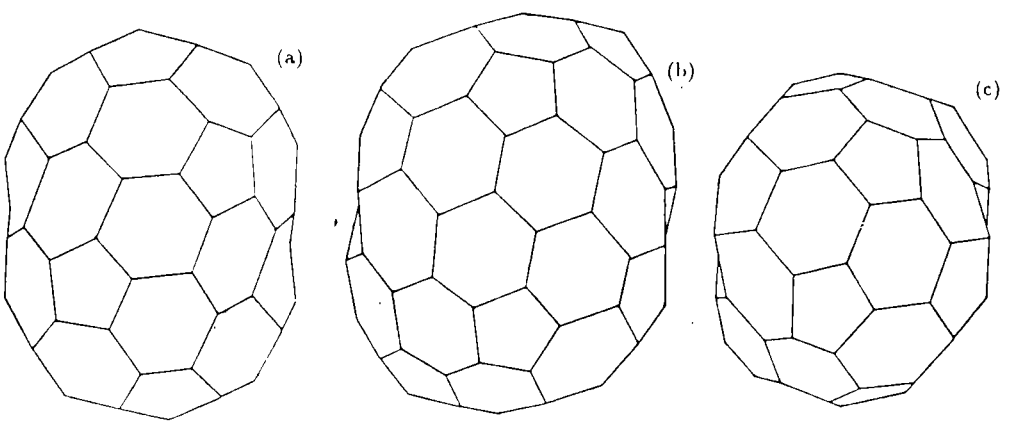


**Fig.1 The structure of $C_{80}$ viewed along each of three symmetry axes of $C_2$**

Soon afterwards it is found that the fold mode would be the key to the question. If the two ends of the structure II is folded upwards and binded at arrows, a $C_{76}$ model can be gotten. But if two ends is folded downwards, a $C_{80}$ model can be gotten only. $C_{76}$ and $C_{80}$ both have the common structural unit-structure I.

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The $C_{80}$ molecule has 3 $C_2$ symmetric axes, which should be vertical each other (see Fig.1). As same as the $C_{76}$ molecule, the $C_{80}$ molecule should have intrinsic helicity of the structure. It should have two chiral allotropes too, and no chiral centre.

$^{13}$C-NMR spectra of $C_{80}$ should consist of 20 lines of equal intensity, corresponding to 20 distinct environments occupied each by four symmetry-equivalent carbon atoms.

$C_{80}$ should be a stable Fullerene molecule. Though there are some helicoid torsion in the molecule, but the bond tension would be small. Up to now, $C_{76}$, $C_{78}$, $C_{82}$, $C_{84}$, $C_{90}$ and $C_{96}$ of the fullerene family have successfully been isolated and indentified[2–5], and their structures, isomers, chiral allotropes have been discussed. But $C_{80}$ has not been reported. However, it should be existent.

## REFERENCES

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